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A NEW, HIGHER-ORDER, ELASTICITY-BASED MICROMECHANICS MODEL

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ABSTRACT: The formulation for a new homogenization theory is presented. The theory utilizes a higher-order, elasticity-based cell analysis of a periodic array of unit cells. The unit cell is discretized into subregions or subcells. The displacement field within each subcell is approximated by an (truncated) eigenfunction function expansion of up to fifth order. The governing equations are developed by satisfying the pointwise governing equations of geometrically linear continuum mechanics exactly up through the given order of the subcell displacement fields. The specified governing equations are valid for any type of constitutive model used to describe the behavior of the material in a subcell. The fifth order theory is subsequently reduced to a third order theory. The appropriate reduction of the fifth and third order theories to the first order theory (which corresponds to a variant of the original method of cells (MOC) (Aboudi, 1991) theory) is outlined. The 3D ECM theory correctly reduces to the 2D ECM theory microstructures and the exact 1D theory for bilaminated structures. Comparison of the predicted bulk and local responses with published results indicates that the theory accurately predicts both types of responses. Furthermore, it is shown that the higher order fields introduced coupling effects between the local fields that can result in substantial changes in the predicted bulk inelastic response of a composite.

KEYWORDS: Multi-scale modeling, homogenization, composite materials, elasticity, plasticity

INTRODUCTION

A current trend in the application of advanced materials is a greater emphasis on understanding the fundamental mechanisms governing the bulk response of the material. There is a multitude of reasons for this focus. As structural applications become more demanding, it is becoming increasingly important that the material microstructure be engineered in order to achieve specific response characteristics. Alternatively, in order to prevent catastrophic failure of a material during service, it is important that the mechanisms that drive the material failure be understood and, at least, predicted and, if possible, countered.

Inherent in the above requirement is the need to address the fact that all materials have microstructure. The heterogeneous nature of material microstructures gives rise to complex interactions at the microstructural level. These interactions can drive critical local and bulk phenomena. Micromechanical theories represent a class of models especially well suited to the analysis of such effects in materials. By their very nature, these models provide predictions for the local behavior in different parts of a material's microstructure as well as providing estimates for the bulk response of a material system. These estimates are obtained by solving the appropriate governing equations of continuum mechanics subject to the constraints of the composite system's microstructural geometry and the response characteristics of the individual components composing a material system. Reviews of many existing micromechanics models are given by Aboudi [1], Christensen [2], and Nemat-Nasser and Hori [3].

The method of cells (MOC) [1] and it's generalization, the generalized method of cells (GMC) [4] have proven to be particularly successful micromechanical theories for modeling both the elastic and inelastic behavior of composite materials. Several studies have shown that the MOC/GMC theories provide accurate estimates for the bulk response of composite systems [5,6]. A review of the work (both elastic and inelastic) conducted using the MOC/GMC theories has been given by Aboudi [7]. Despite the demonstrated ability of the MOC/GMC theories to model the bulk response of composites, a major issue in the use of the these models is the lack of coupling between the local shearing and normal effects as well as between local shearing effects of different types. This lack has implications for the history-dependent analysis of composite materials. In particular, this lack can result in incorrect evolution of local history-dependent phenomena and, hence, of the bulk history-dependent behavior of the composite.

The purpose of the present paper is to present the development of a new type of higher-order, elasticity-based theory (denoted as ECM for elasticity-based, cell model) for homogenization analyses that rectifies the issue of the lack of coupling between the local fields. The proposed theory is based on the assumption of periodic arrays of inclusions (either doubly or triply periodic arrays). The resulting unit cells are discretized into subcells in a manner similar to that used by the original MOC. The displacement field within each subcell is approximated by a (truncated) eigenfunction expansion of up to fifth order. The strong form of the point wise governing equations of geometrically linear continuum mechanics are satisfied exactly up through an order consistent with the order of the subcell displacement fields. In particular, the formulation satisfies the equations of equilibrium within the subcells and the traction and displacement continuity constraints both between subcells and between unit cells. The theory is formulated independently of the material constitutive relations for the individual phases and, thus, can any type of (geometrically linear strain) constitutive theory. It is shown that the theory accurately predicts the bulk elastic properties for continuous fiber and particulate composites. Additionally, the application of the current theory to inelastic deformation problems is considered.

THEORETICAL FRAMEWORK

This section outlines the development of the framework for the three-dimensional, 5th (cumulative) order version of the elasticity-based, cell model (ECM). The following conventions are used throughout the formulation. Summation is implied on Arabic subscripts and superscripts. An overbar denotes a mean (volume averaged) field where for a generic field F this mean field is given by $\overline{F} = \frac{1}{V}\int F dV$ where V is the volume of the unit cell.

Consider a triply periodic array of inclusions embedded in a matrix, Fig. 1. The composite system is subjected to a homogeneous displacement field $U_i = \overline{\varepsilon}_{ij} x_j$ where the $\overline{\varepsilon}_{ij}$ are the bulk (average) strains in the composite and the x_j are the macroscopic coordinates in the composite. Implied by this type of material microstructure and global loading state is the fact that it is sufficient to analyze only a single repeating unit cell (Fig. 1). This unit cell is subdivided into eight subregions or subcells. The superscript (αβγ) is used to denote the subcell within the unit cell where α, β, and γ range from 1 to 2 individually. A local coordinate system $\overline{x}_i$ is defined at the center of each subcell.

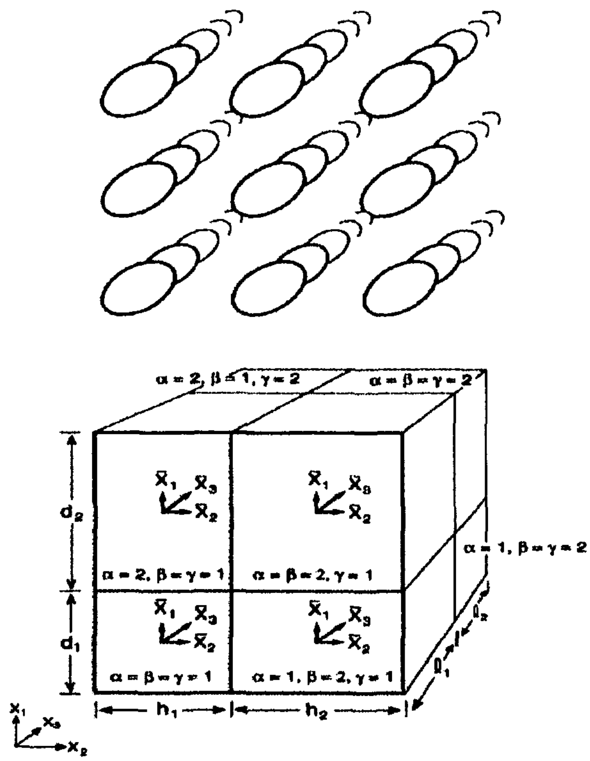


Figure 1: The triply periodic array of inclusions and the corresponding discretized unit cell employed in the current analysis.

The assumed subcell displacement field is

$$u_{i(mnr)}^{(\alpha\beta\gamma)} = \overline{\varepsilon}_{ij} x_j + P_{(mnr)} V_{i(mnr)}^{(\alpha\beta\gamma)}$$

where

$$P_{(mnr)} = p_m(\bar{x}_1)p_n(\bar{x}_2)p_r(\bar{x}_3)$$

and the $p_m(\bar{x}_l)$ are dimensional Legendre polynomials of order m in the local subcell coordinate $\bar{x}_l$, m takes the values 1, 3 or 5, and the cumulative order $m+n+r$ must also be 1, 3, or 5. The $V_{i(mnr)}^{(\alpha\beta\gamma)}$ are the material microstructure induced fluctuating displacement field effects about the applied homogeneous displacement field. There are 102 unknown $V_{i(mnr)}^{(\alpha\beta\gamma)}$ per subcell or 816 unknowns per unit cell. The even (cumulative) order displacement terms are not considered since they decouple from the odd (cumulative) order and hence are identically zero. Based on the geometrically linear definition of strain the subcell strains take the following functional form

$$\varepsilon_{ij}^{(\alpha\beta\gamma)} = P_{(pqs)}\varepsilon_{ij(pqs)}^{(\alpha\beta\gamma)} = P_{(000)}\bar{\varepsilon}_{ij} + P_{(pqs)}\mu_{ij(pqs)}^{(\alpha\beta\gamma)}$$

where p, q, s take the values 0, 2, or 4 individually and the cumulative order $p+q+s$ must take the values 0, 2, or 4. The $\mu_{ij(pqs)}^{(\alpha\beta\gamma)}$ represent the fluctuating strain effects. The corresponding subcell stress field is

$$\sigma_{ij}^{(\alpha\beta\gamma)} = P_{(pqs)}\sigma_{ij(pqs)}^{(\alpha\beta\gamma)}$$

Any set of desired constitutive relations can be used to relate the strain field to the stress field.

The governing equations for the theory are obtained by satisfying the strong form of the displacement and traction continuity conditions across each interface

$$[u_i] = 0$$

$$[\sigma_{ij}n_i] = 0$$

(where $[F]$ denotes the jump in field F across the interface) as well as the point wise equilibrium equations within each subcell

$$\partial_1\sigma_{1i} + \partial_2\sigma_{2i} + \partial_3\sigma_{3i} = 0$$

where ∂_i denotes partial differentiation with respect to the x_i coordinate. Due to periodicity and the particular forms for the local fields the continuity conditions simultaneously satisfy the continuity conditions both within and between unit cells.

Substituting the local fields for the displacements and stresses in the subcells into the above governing equations for continuum mechanics and using the orthogonality properties of the expansion functions $p_m(\overleftarrow{x}_i)$ provides the governing equations for the theory. The resulting system of governing equations is appropriate for any particular set of constitutive models for the material behavior. To obtain the final form for the governing equations it is necessary to assume a particular set of constitutive relations for the materials occupying the subcells. For this work the following form for the constitutive relations for the materials composing each subcell are assumed

$$\sigma = C(\varepsilon - e)$$

where C is the stiffness tensor, ε is the total strain, and e represents the eignestrain effects. The evolution law for the eigenstrains (in this case inelastic strains) is given by

$$e = \lambda s$$

where λ is the proportionality factor, and s is the stress deviations. The proportionality factor λ is calculated using either classical incremental plasticity theory (Williams and Pindera [10]) or the Bodner-Partom (BP) unified viscoplastic theory [11]. Substituting this form for the constitutive relations into the governing equations allows these governing equations to be written in the following matrix form

$$\underline{\underline{K}}\underline{V} = \underline{\underline{F}}\,\underline{\bar{\varepsilon}} + \underline{\underline{h}}\,\underline{e}$$

where $\underline{\underline{K}}$, $\underline{\underline{F}}$, and $\underline{\underline{h}}$ are coefficient matrices that are known functions of the material properties and the microstructural geometry and $\underline{e}$ is a vector composed of the eigenstrain effects within the subcells. The details of the governing equations are given by Williams [8,9]. The third order theory is obtained by eliminating all 5th (cumulative) order terms in the displacement expansion and all 4th (cumulative) order terms in the strain and stress expansions as well as the associated governing equations. The reduction to the 1st order theory follows a similar process. To reduce the 3D theory to the 2D theory the spatial dependencies with respect to one direction are eliminated from the analysis. The details of these reductions to lower order theories are given in detail by Williams [8,9].

RESULTS

A necessary condition for the validation of the model is that it correctly reduces to the lower order theories (i.e. 1st and 3rd order theories) as well as the lower order dimensionalities. The 5th order model presented above does correctly reduce to both the analyses based on lower order expansions for the fields as well as the 2D and 1D cases. It is noted that the 1D result represents an exact solution for a bilaminate (Aboudi [1]). For conciseness, these results are not presented.

First, the theory's ability to predict the effective elastic moduli is considered. The predictions from the 3rd order ECM, the MOC model, and various finite element analyses [6,12] for the effective transverse shear modulus of a Gr/Ep composite are given, Fig. 2. The elastic properties for the (Modmor II) Gr fiber are E_l=232.0 GPa, E_t=15.0 GPa, ν_{tt}=0.49, ν_{lt}=0.279, G_{tt}=5.03 GPa, and G_{lt}=24.0 GPa and the corresponding properties for the LY558 epoxy are E=5.35 GPa, ν=0.354, G=1.976 GPa [6]. The extreme contrast in the material properties represents a stringent test of a micromechanical theory's ability to correctly predict the effective properties of a composite. The ECM predictions are in excellent agreement with the finite element predictions based on a square array of fibers [6] and are more accurate than the MOC predictions.

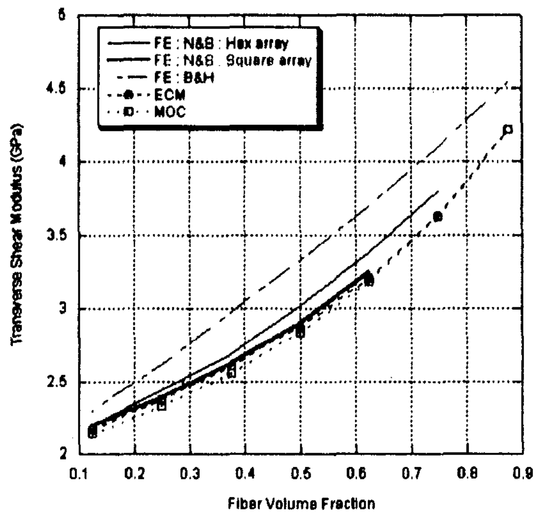
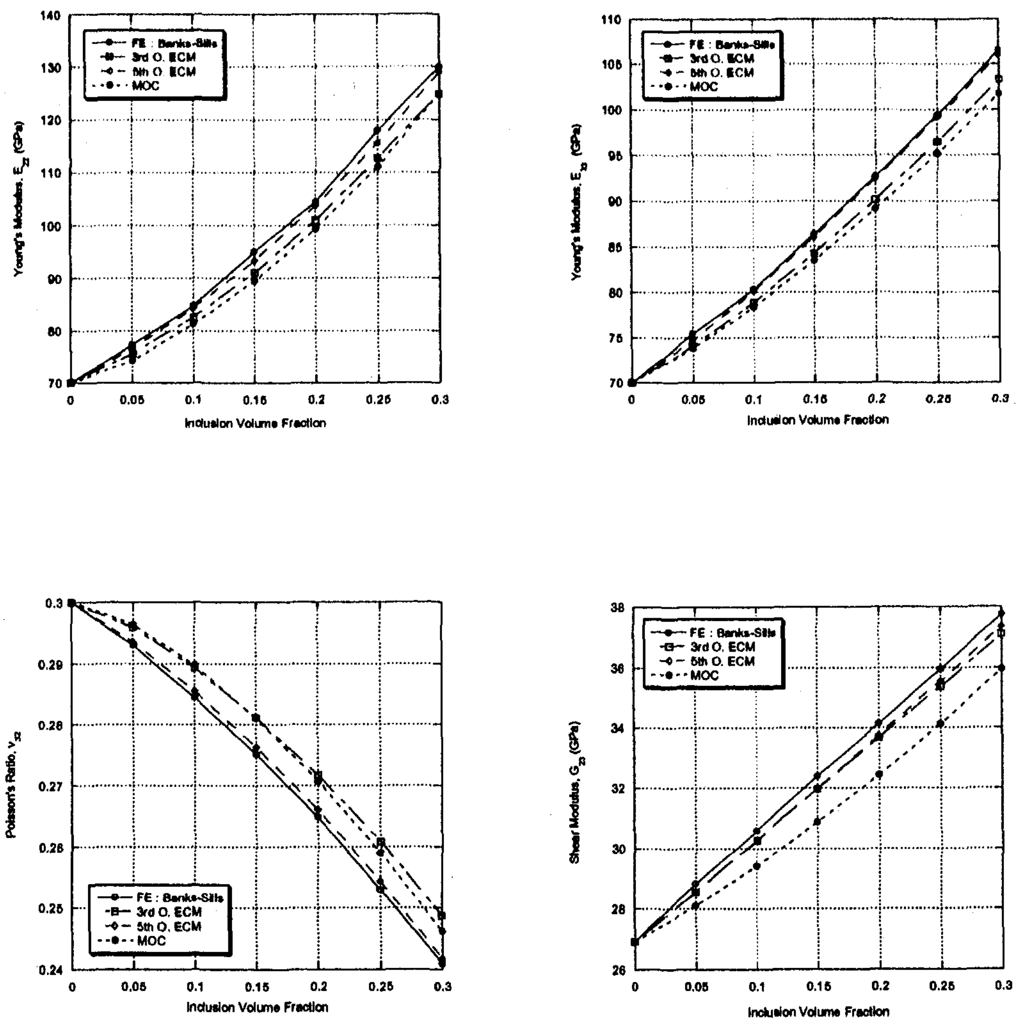


Figure 2: Predictions for the effective transverse shear modulus of a Gr/Ep continuous fiber composite obtained from different finite element analysis, the 3rd order ECM theory, and the MOC model.

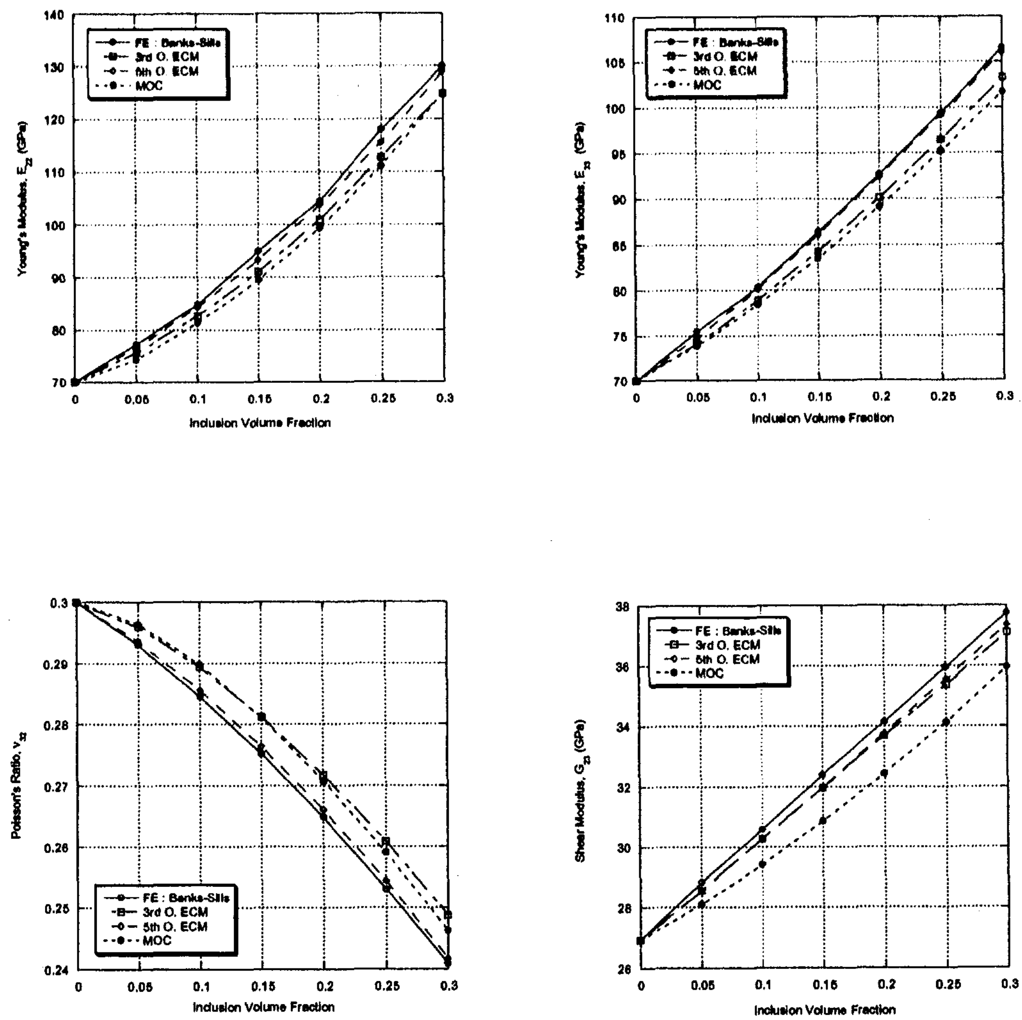
It is noted that the present theory is also able to correctly predict the local fields in a 2D composite (not shown) [8,9].

Next, the predictions for E_{22}, E_{33}, ν_{32}, and G_{23} as a function of inclusion volume fraction obtained from the 5th and 3rd order ECM are compared to predictions obtained from the MOC model and the results generated by Banks-Sills *et. al.* [13] for a particulate composite system composed of a rectangular parallelepiped Al_2O_3 inclusion (Young's modulus of 350 GPa and a Poisson's ratio of 0.30) embedded in an aluminum matrix (Young's modulus of 70 GPa and a Poisson's ratio of 0.30) is presented, Fig. 3-7. The results of Banks-Sills *et. al.* [13] are derived by using the asymptotic homogenization theory (Bensoussan *et. al.* [14]) in conjunction with highly detailed finite element simulations of the unit cell. In the following discussion, this approach is referred to as the HFE method. As can be seen both the 5th and 3rd order ECM provide high fidelity predictions of the bulk response of this particulate composite system with the 5th order theory providing the more accurate predictions. The MOC model provides the least accurate predictions for the effective behavior. The improvement in the predictions for the effective G_{23} from the ECM as compared to those obtained from the MOC theory are particularly noteworthy. The high degree of agreement between the current theory results and HFE results as compared to the correlation between the MOC and HFE results is due to the correct incorporation of the coupling effects between the local fields in the ECM. Furthermore, it is noted that the ECM employs substantially fewer unknowns in the analysis than does the HFE method and, hence, the ECM is more computational efficient.



Figures 3-6: The predictions for the effective E_{22}, E_{33}, ν_{32}, and G_{23} as function of inclusion volume fraction for an Al_2O_3/Al composite with rectangular parallelepiped inclusions.

Now the inelastic response of an Al_2O_3/Al composite with cubic inclusions with a volume fraction of 0.3 is considered. The elastic properties of the phases used in the analyses are those for the effective behavior. The improvement in the predictions for the effective G_{23} from the ECM as compared to those obtained from the MOC theory are particularly noteworthy. The high degree of agreement between the current theory results and HFE results as compared to the correlation between the MOC and HFE results is due to the correct incorporation of the coupling effects between the local fields in the ECM. Furthermore, it is noted that the ECM employs substantially fewer unknowns in the analysis than does the HFE method and, hence, the ECM is more computational efficient.



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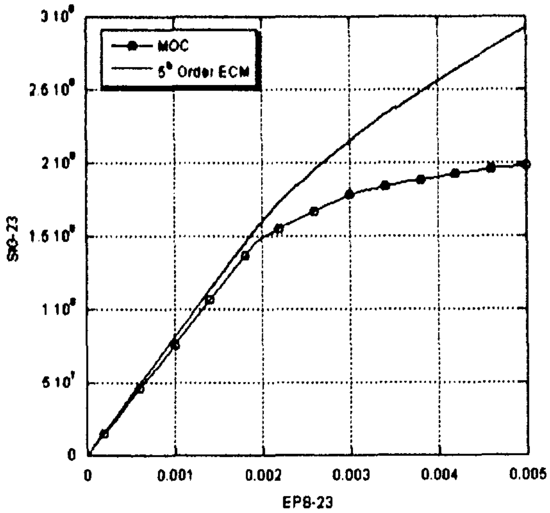

Figure 8: Predicted bulk shear response of an Al_2O_3/Al particulate composite with cubic inclusions.

Most of the trends observed in the normal macroscopic stress-strain responses are also present in the bulk shear response of the composite. In particular, the MOC results exhibit the abrupt transition from the elastic to the inelastic behavior previously observed with the subsequent inelastic behavior rapidly saturating. The transition from the elastic to the inelastic responses predicted by the ECM is substantially more gradual than the corresponding MOC regime. This slower evolution of the bulk inelastic response results in substantially increased macroscopic stresses in the ECM response as compared to the MOC response. The explanations for these differences again resides in the fact that the MOC model yields entire regions within the microstructure simultaneously while the ECM predicts that yielding occurs in a point wise fashion. Consideration of the microfields predicted by the ECM shows that at for strains where the MOC model exhibits saturated inelastic behavior the local ECM fields still exhibit regions of completely elastic deformations, i.e. regions where yielding has not occurred. Additionally, the local plastic strain fields in the subcells exhibit extreme localization effects.

SUMMARY

The development of a new homogenization theory for 2D and 3D composite materials has been presented. The theory is based on a displacement based elasticity analysis of a repeating unit cell. The displacement field within each subcell has been expressed in terms of a 5^{th} (cumulative) order eigenfunction expansion. The analysis satisfies the strong (point wise) form of the governing equations of geometrically linear continuum mechanics. The resulting formulation correctly introduces coupling between the local fields (both normal and shearing) within the subcells. The theory is formulated based on arbitrary material behavior within the subcells and hence any desired set of constitutive theories for the behavior of the materials in the subcells can be implemented.

The theory has been shown to accurately predict the bulk behavior of both continuous fiber and particulate composite systems. Additionally, it has been shown that the incorporation of coupling between the local normal and shearing effects within the subcells can substantially influence the predicted bulk inelastic response of a composite as compared to analyses where the local fields are not coupled. In particular, the evolution of the predicted bulk inelastic response is more gradual in the ECM than in the MOC. Due to this delayed evolution of the bulk inelastic deformations, the ECM predicts substantially different macroscopic stress states in the inelastic regime than does with the MOC model.

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